

<b>L Number</b>	<b>Hits</b>	<b>Search Text</b>	<b>DB</b>	<b>Time stamp</b>
<b>1</b>	<b>367</b>	<b>("568/648").CCLS.</b>	<b>USPAT; US-PGPUB; EPO; JPO; DERWENT</b>	<b>2001/09/20 08:27</b>
<b>2</b>	<b>0</b>	<b>1-propyl-2,4,5-trimethoxybenzene</b>	<b>USPAT; US-PGPUB; EPO; JPO; DERWENT</b>	<b>2001/09/20 08:29</b>
<b>3</b>	<b>0</b>	<b>"1-propyl-2,4,5-trimethoxybenzene"</b>	<b>USPAT; US-PGPUB; EPO; JPO; DERWENT</b>	<b>2001/09/20 08:29</b>
<b>4</b>	<b>0</b>	<b>1-propyl near2 "2,4,5-trimethoxybenzene"</b>	<b>USPAT; US-PGPUB; EPO; JPO; DERWENT</b>	<b>2001/09/20 08:33</b>
<b>5</b>	<b>1</b>	<b>"2,4,5-trimethoxybenzene"</b>	<b>USPAT; US-PGPUB; EPO; JPO; DERWENT</b>	<b>2001/09/20 08:30</b>
<b>6</b>	<b>243</b>	<b>calamus or \$6asarone</b>	<b>USPAT; US-PGPUB; EPO; JPO; DERWENT</b>	<b>2001/09/20 08:32</b>
<b>7</b>	<b>1</b>	<b>((("568/648").CCLS.) and ( calamus or \$6asarone )</b>	<b>USPAT; US-PGPUB; EPO; JPO; DERWENT</b>	<b>2001/09/20 08:32</b>
<b>8</b>	<b>447</b>	<b>\$trimethoxybenzene</b>	<b>USPAT; US-PGPUB; EPO; JPO; DERWENT</b>	<b>2001/09/20 08:33</b>
<b>9</b>	<b>15</b>	<b>\$trimethoxybenzene and (((("568/648").CCLS.) or ( calamus or \$6asarone ))</b>	<b>USPAT; US-PGPUB; EPO; JPO; DERWENT</b>	<b>2001/09/20 08:38</b>
<b>10</b>	<b>0</b>	<b>"2,4,5-trimethoxybenzene" and ( calamus or \$6asarone )</b>	<b>USPAT; US-PGPUB; EPO; JPO; DERWENT</b>	<b>2001/09/20 08:38</b>

09/652,376

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TOTAL

ENTRY

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FULL ESTIMATED COST

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0.15

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STRUCTURE FILE UPDATES: 18 SEP 2001 HIGHEST RN 357383-23-4

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Please note that search-term pricing does apply when conducting SmartSELECT searches.

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=>

Uploading C:\STNEXP4\QUERIES\09652376.str

L1        STRUCTURE UPLOADED

=> que L1

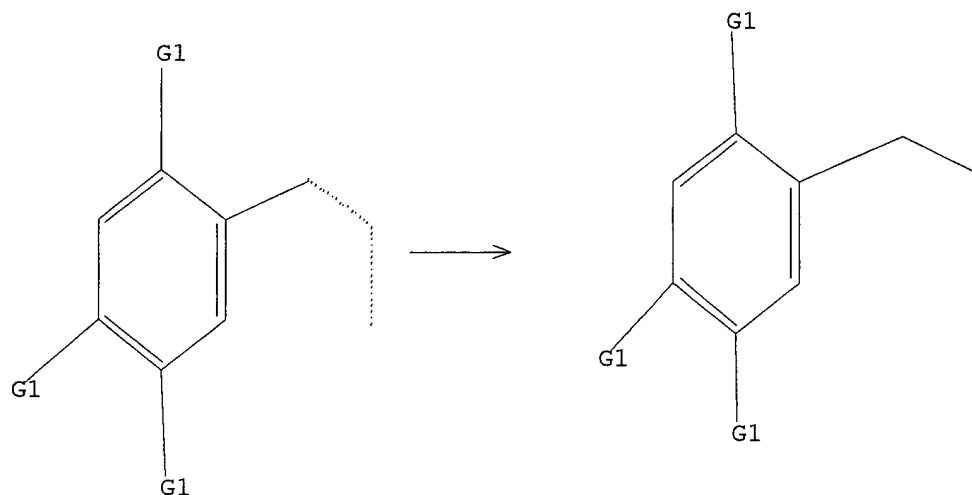
L2    QUE L1

=> d

L2 HAS NO ANSWERS

L1                STR

09/652,376



G1 MeO, EtO, n-PrO, i-PrO, n-BuO, i-BuO, s-BuO, t-BuO

Structure attributes must be viewed using STN Express query preparation.  
L2 QUE L1

=> file reaction

COST IN U.S. DOLLARS

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TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.62

0.77

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=> s 12

SAMPLE SEARCH INITIATED 09:24:58 FILE 'CASREACT'  
SCREENING COMPLETE - 441 REACTIONS TO VERIFY FROM

60 DOCUMENTS

100.0% DONE 441 VERIFIED 0 HIT RXNS  
SEARCH TIME: 00.00.05

0 DOCS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED VERIFICATIONS: 7562 TO 10078  
PROJECTED ANSWERS: 0 TO 0

SAMPLE SEARCH INITIATED 09:25:04 FILE 'CHEMINFORMRX'

09/652,376

SCREENING COMPLETE - 45 REACTIONS TO VERIFY FROM 21 DOCUMENTS  
100.0% DONE 45 VERIFIED 0 HIT RXNS 0 DOCS  
SEARCH TIME: 00.00.05

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED VERIFICATIONS: 498 TO 1302  
PROJECTED ANSWERS: 0 TO 0

SAMPLE SEARCH INITIATED 09:25:11 FILE 'CHEMREACT'  
SCREENING COMPLETE - 7 REACTIONS TO VERIFY FROM 7 DOCUMENTS  
100.0% DONE 7 VERIFIED 0 HIT RXNS 0 DOCS  
SEARCH TIME: 00.00.03

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED VERIFICATIONS: 7 TO 149  
PROJECTED ANSWERS: 0 TO 0

3 FILES SEARCHED...  
FULL SEARCH INITIATED 09:25:17 FILE 'DJSMONLINE'  
SCREENING COMPLETE - 46 REACTIONS TO VERIFY FROM 36 DOCUMENTS  
100.0% DONE 46 VERIFIED 0 HIT RXNS 0 DOCS  
SEARCH TIME: 00.00.04

L3 0 L2

=> s l2 ful  
FULL SEARCH INITIATED 09:25:28 FILE 'CASREACT'  
SCREENING COMPLETE - 12589 REACTIONS TO VERIFY FROM 1354 DOCUMENTS  
100.0% DONE 12589 VERIFIED 32 HIT RXNS 11 DOCS  
SEARCH TIME: 00.00.08

FULL SEARCH INITIATED 09:25:41 FILE 'CHEMINFORMRX'  
SCREENING COMPLETE - 1804 REACTIONS TO VERIFY FROM 594 DOCUMENTS  
100.0% DONE 1804 VERIFIED 9 HIT RXNS 4 DOCS  
SEARCH TIME: 00.00.23

2 FILES SEARCHED...  
FULL SEARCH INITIATED 09:26:06 FILE 'CHEMREACT'  
SCREENING COMPLETE - 189 REACTIONS TO VERIFY FROM 189 DOCUMENTS  
100.0% DONE 189 VERIFIED 1 HIT RXNS 1 DOCS  
SEARCH TIME: 00.00.10

FULL SEARCH INITIATED 09:26:18 FILE 'DJSMONLINE'  
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100.0% DONE 46 VERIFIED 0 HIT RXNS 0 DOCS  
SEARCH TIME: 00.00.02

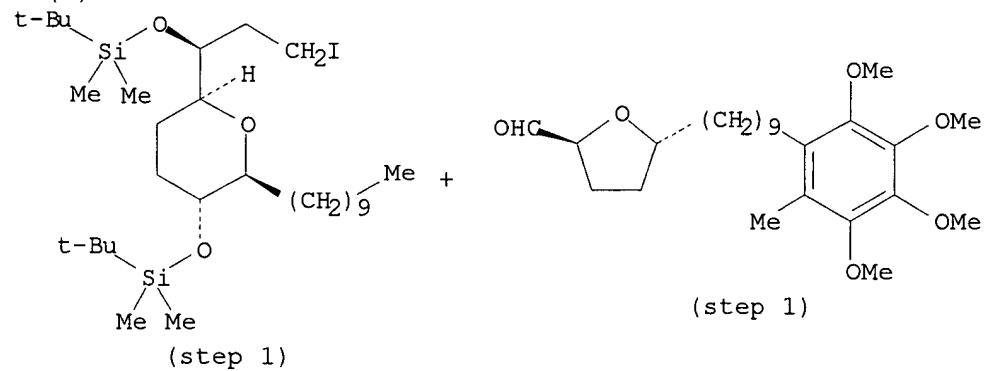
L4 16 L2

09/652,376

=> d 1-16

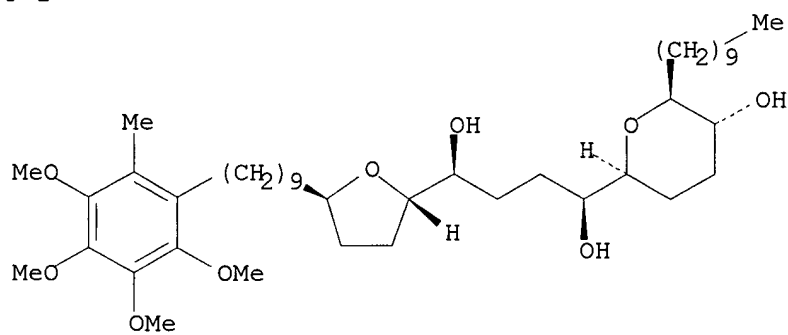
L4 ANSWER 1 OF 16 CASREACT COPYRIGHT 2001 ACS

RX(1) OF 1



1. BuLi, MgBr<sub>2</sub>-Et<sub>2</sub>O,  
Et<sub>2</sub>O  
2. HF, CH<sub>2</sub>Cl<sub>2</sub>, MeCN →

RX(1) OF 1



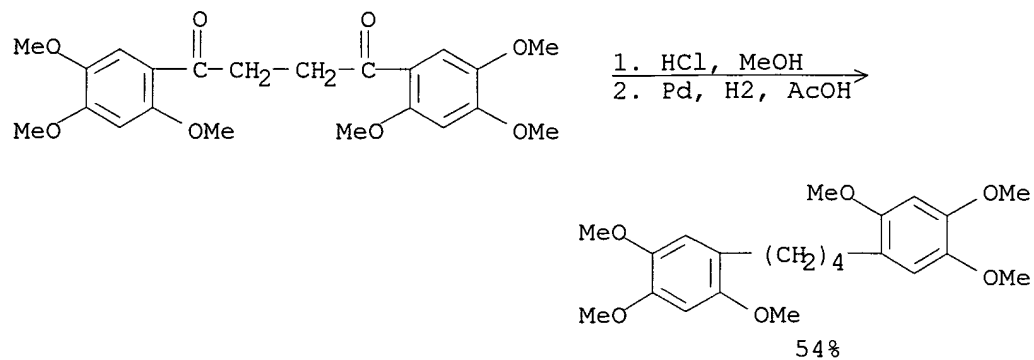
90%

REF: Angew. Chem., Int. Ed., 39(12), 2099-2102; 2000

L4 ANSWER 2 OF 16 CASREACT COPYRIGHT 2001 ACS

09/652,376

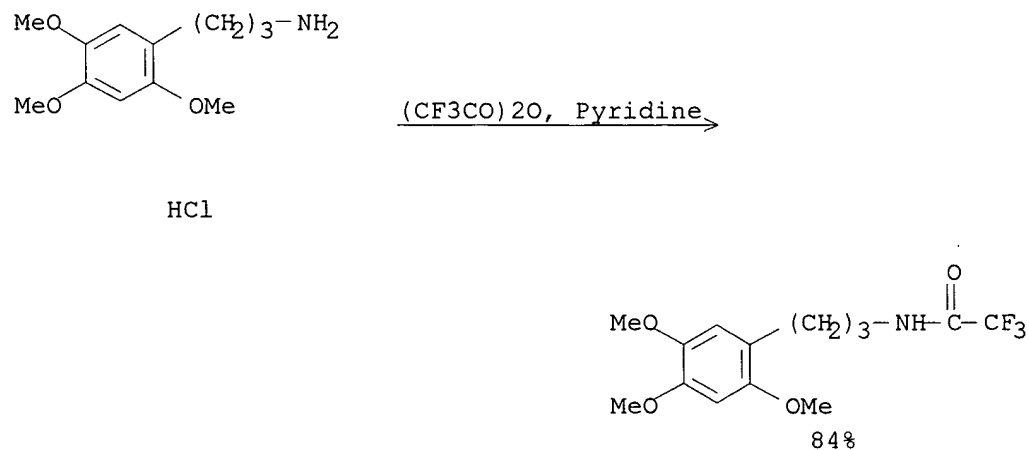
RX(7) OF 10 - 2 STEPS



REF: Org. Prep. Proced. Int., 24(1), 78-80; 1992

L4 ANSWER 3 OF 16 CASREACT COPYRIGHT 2001 ACS

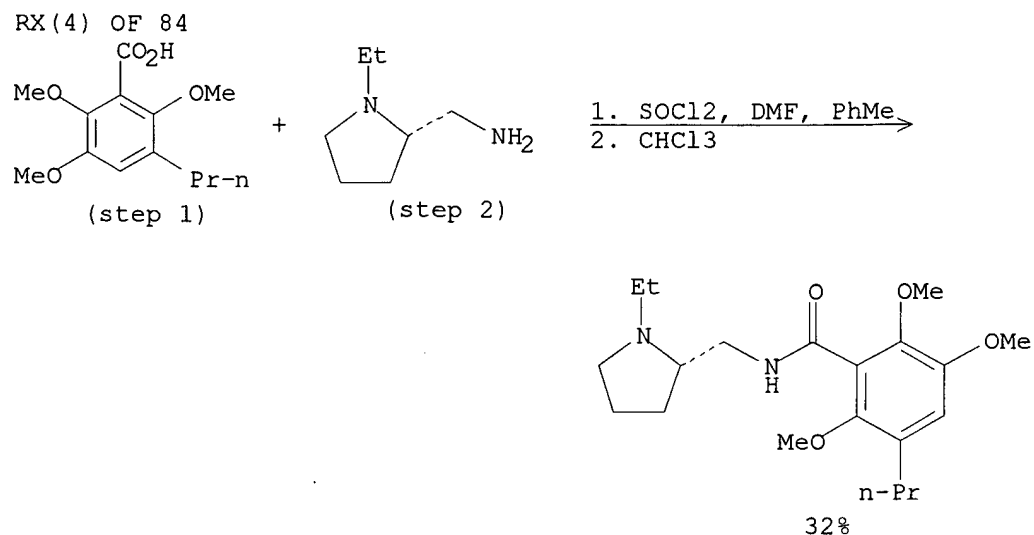
RX(5) OF 257



REF: J. Org. Chem., 55(7), 2019-26; 1990

L4 ANSWER 4 OF 16 CASREACT COPYRIGHT 2001 ACS

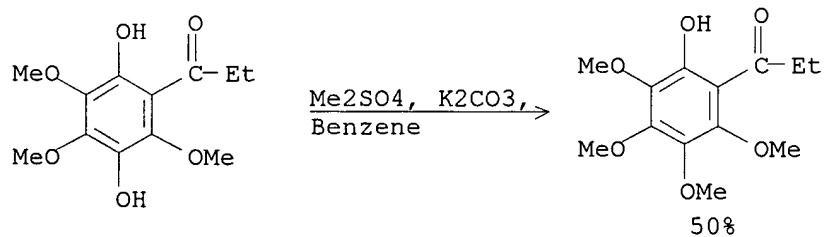
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REF: J. Med. Chem., 33(4), 1155-63; 1990

L4 ANSWER 5 OF 16 CASREACT COPYRIGHT 2001 ACS

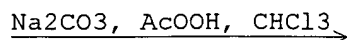
RX(1) OF 20



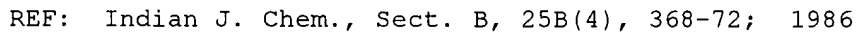
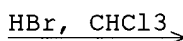
REF: Tetrahedron Lett., 29(19), 2347-8; 1988

L4 ANSWER 6 OF 16 CASREACT COPYRIGHT 2001 ACS

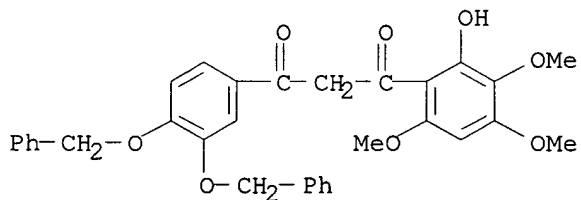
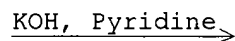
RX (12) OF 51



RX (2) OF 13



RX (65) OF 540



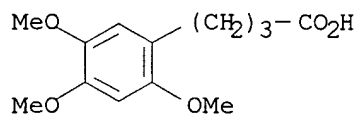
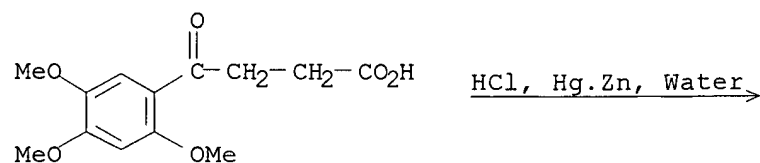
REF: J. Med. Chem., 29(11), 2256-62; 1986

L4 ANSWER 9 OF 16 CASREACT COPYRIGHT 2001 ACS



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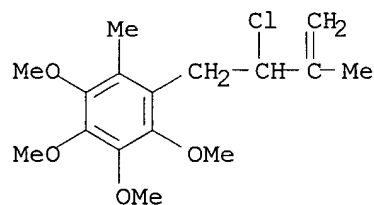
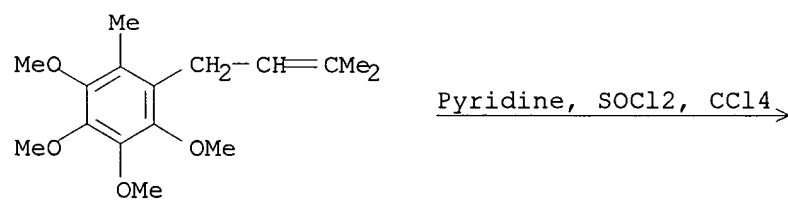
RX(1) OF 243



REF: Helv. Chim. Acta, 68(8), 2324-31; 1985

L4 ANSWER 10 OF 16 CASREACT COPYRIGHT 2001 ACS

RX(8) OF 411

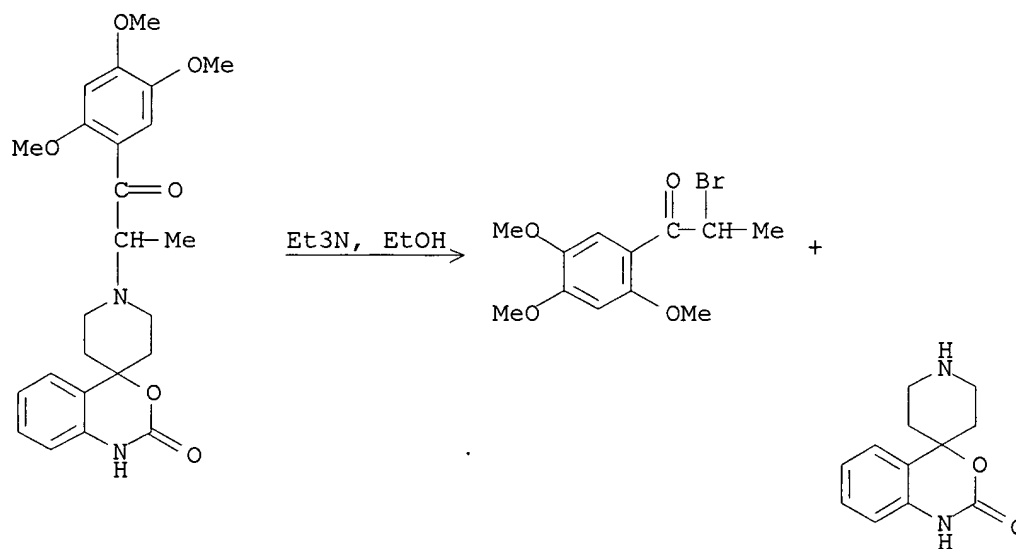


REF: Chem. Pharm. Bull., 33(5), 1930-40; 1985

L4 ANSWER 11 OF 16 CASREACT COPYRIGHT 2001 ACS

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RX(28) OF 365

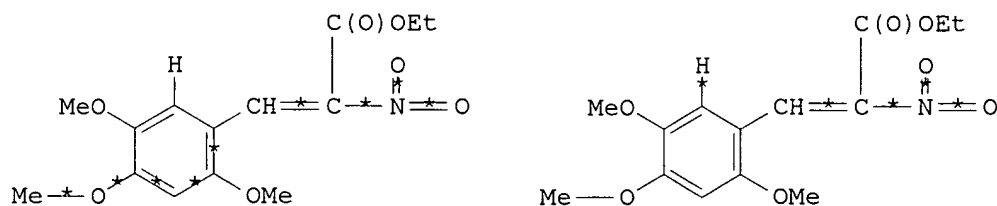


HCl

REF: Chem. Pharm. Bull., 33(3), 1129-39; 1985

L4 ANSWER 12 OF 16 CHEMINFORMRX COPYRIGHT 2001 FIZ CHEMIE  
 199934151 A Facile Synthesis of Spiroisoxazolines: Intramolecular  
 Cyclization of 3-Aryl-2-nitroacrylates Promoted by Titanium  
 Tetrachloride. HIROTANI, S.; KAJI, E. Sch. Pharm. Sci., Kitasato  
 Univ., Minato, Tokyo 108, Japan Tetrahedron, 55(14), 4255-4270,  
 (1999)  
 CODEN: TETRAB ISSN: 0040-4020 English

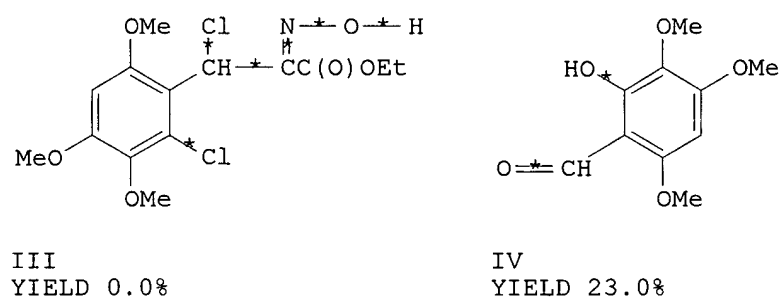
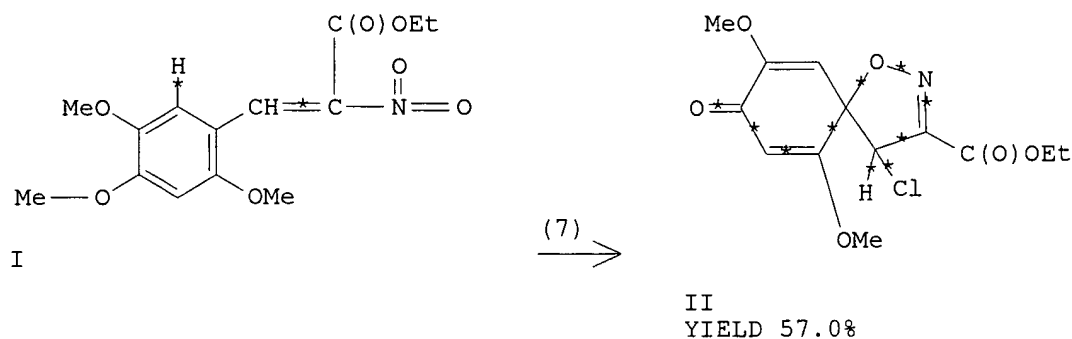
RX(7) OF 10 3 I ==> II + III + IV



I

I

09/652,376



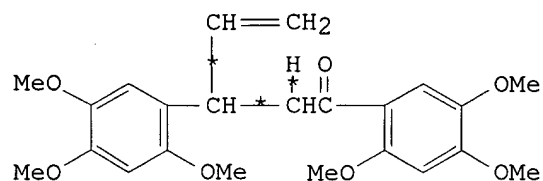
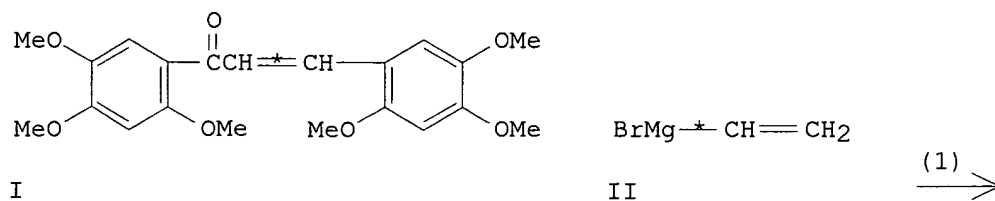
RX(7) RCT I, **691620**  
 RGT 1151 (7550-45-0), TiCl<sub>4</sub>  
 SOL 60 (75-09-2), CH<sub>2</sub>Cl<sub>2</sub>  
 PRO II, 691621  
 III, **691622**  
 IV, 691623  
 YDS 80.0 %  
 T 0.0 Cel  
 TIM 24 hr  
 KW dearomatisation; halogenation; C-halogenation; chlorination;  
 alkylation; O-alkylation; arylation; O-arylation  
 NTE reaction: I -> II + III + IV, example: 7  
 CMT #E0100:(isom. mix.)

L4 ANSWER 13 OF 16 CHEMINFORMRX COPYRIGHT 2001 FIZ CHEMIE  
 199506129 Chalcones as Synthetic Intermediates. A Facile Route to  
 (.-.-.)-

Magnosalicin, an Antiallergy Neolignan. MURAOKA, O.; SAWADA, T.;  
 MORIMOTO, E.; TANABE, G. Fac. Pharm. Sci., Kinki Univ.,  
 Higashi-Osaka, Osaka 577, Japan Chem. Pharm. Bull., 41(4), 772-774,  
 (1993)  
 CODEN: CPBTAL ISSN: 0009-2363 English

RX(1) OF 15 I + II ==> III...

09/652,376



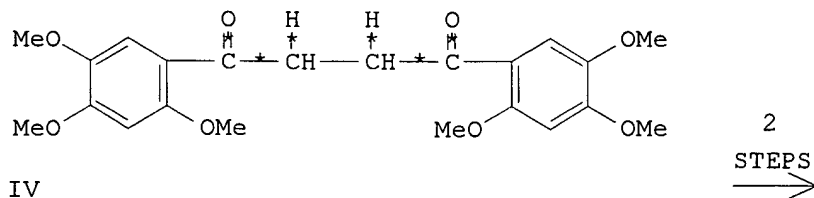
III  
YIELD 78.0%

RX(1)      RCT    I, **361621**  
                      II, 1329 (1826-67-1)  
                      RGT    1145 (7681-65-4), CuI  
                      SOL    206 (109-99-9), THF  
                      PRO    III, **361622**  
                      YDS    78.0 %  
                      T      0.0 Cel  
                      KW    Grignard reaction; addition; alkylation; C-alkylation  
                      NTE    reaction:I (II) -> III  
                      CMT    Ratio = 3:1 for products 1,2

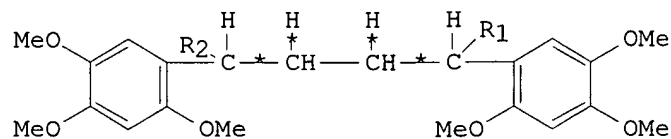
L4    ANSWER 14 OF 16 CHEMINFORMRX    COPYRIGHT 2001 FIZ CHEMIE  
      199236138    Preparation of 1,4-Bis(2,4,5-trimethoxyphenyl)butane.  
                      AL-FARHAN, E.; AMOFAH, R.; KEEHN, P. M.; STEVENSON, R.    Dep. Chem.,  
                      Brandeis Univ., Waltham, MA 02254-9110, USA    Org. Prep. Proced.

Int.,  
      24(1), 78-80, (1992)  
      CODEN: OPPIAK    ISSN: 0030-4948    English

RX(7) OF 10 COMPOSED OF RX(3), RX(4)  
RX(7)      **IV** ==> **VI**



09/652,376



VI  
YIELD 54.0%

RX(3) RCT IV, **66116** (139452-24-7)  
RGT 103 (7647-01-0), HCl  
SOL 123 (67-56-1), MeOH  
PRO V, 66117 (139452-23-6)  
YDS 98.0 %  
T.KW REFLUX  
TIM 1.0 hr  
KW alkylation; O-alkylation; etherification  
NTE reaction:IV -> V  
RX(4) RCT V, 66117 (139452-23-6)  
RGT 107 (1333-74-0), H2  
SOL 3 (64-19-7), AcOH  
CAT 1237 (71717-87-8), Pd-C  
PRO VI, **66118** (139452-22-5)  
YDS 54.0 %  
T 25.0 Cel  
TIM 16 hr  
NTE reaction:V -> VI

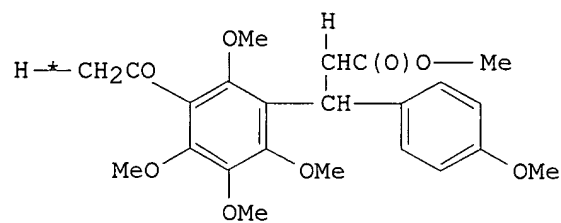
L4 ANSWER 15 OF 16 CHEMINFORMRX COPYRIGHT 2001 FIZ CHEMIE  
199117232 Synthesis of

5'-(1-(Methoxycarbonyl)-2-(p-methoxyphenyl)ethyl)-  
and 5'-

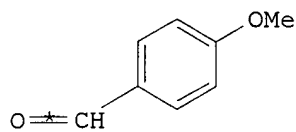
(2-(Methoxycarbonyl)-1-(p-methoxyphenyl)ethyl)-2',3',4,4',6'-  
pentamethoxychalcone. OBARA, H.; ONODERA, J.; TSUCHIYA, M.;  
MATSUEDA, H.; SATO, S.; MATSUBA, S. Dep. Mater. Sci. Eng., Fac.  
Eng., Yamagata Univ., Yonezawa 992, Japan Bull. Chem. Soc. Jpn.,  
64(1), 309-311, (1991)  
CODEN: BCSJA8 ISSN: 0009-2673 English

RX(4) OF 6 ...**XI** + XII + XIII ==> **XIV**

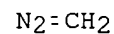
09/652,376



XI

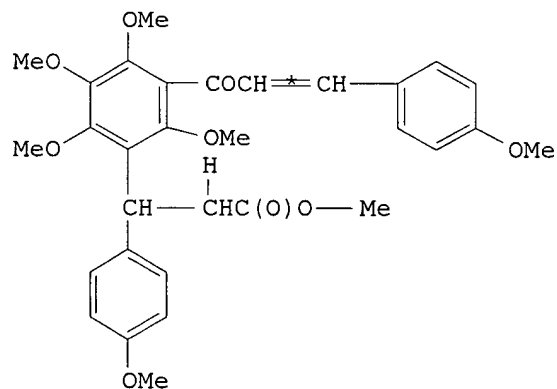


XII



XIII

(4)  $\longrightarrow$



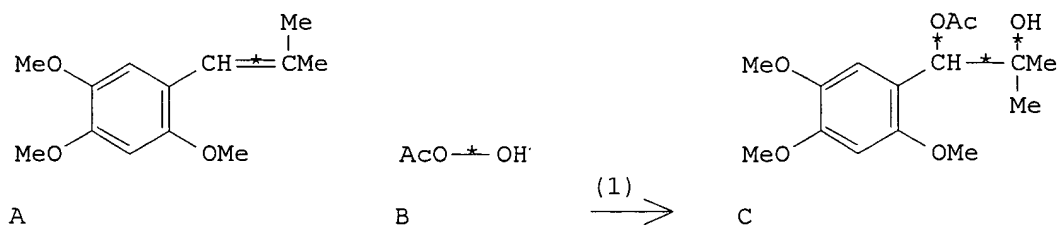
XIV

YIELD 90.0%

RX(4) RCT XI, **148788** (133466-29-2)  
 XII, 8423 (123-11-5)  
 XIII, 49 (334-88-3)  
 STAGE(1)  
 RGT 1160 (1310-58-3), KOH  
 SOL 123 (67-56-1), MeOH  
 YDS 90.0 %  
 STAGE(2)  
 SOL 61 (60-29-7), Et2O  
 YDS 100.0 %  
 PRO XIV, **148789** (126094-00-6;133574-63-7)  
 YDS 90.0 %  
 KW olefination  
 NTE reaction:XI 1.(XII) 2.(XIII) -> XIV  
 CMT Ratio = 75:25 for products 1,2

L4 ANSWER 16 OF 16 CHEMREACT COPYRIGHT 2001 SPRINGER/IC  
 RX(1) OF 1 A + B ==> C

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=> file stnguide

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LAST RELOADED: Sep 14, 2001 (20010914/UP).

=> file chemistry patent

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COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

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0.00

255.66

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